Name: _____

PHYSICS 619 : SPRING SEMESTER 2019

Project #5: Molecular Dynamics Simulations

Modify the MD program using the VV algorithm so that it can simulate up to 27 argon atoms. (i.e., dimension your position, velocity arrays, etc., up to 27.) Set up the program so that it can read in NP (number of particles), DT (time step size), NITER (number of time-step iteration), and the NP set of initial positions and velocities of the particles. Divide your program at least into three parts. The main program for reading in initial data and outputing results. The subroutine ACCEL for computing the the acceleration of all particles given their current positions. The subroutine UPDATE for updating all particle positions one time-step forward. Initially, do it only for two-dimension in a periodic box with $SX = SY = 10$. All distance are measured in units of σ and all particles effectively have unit masses. You must call ACCEL once before the start of your updating loop.

1.) To check your program, do the following very simple run. Let particle 1 be initially resting at (7.0, 6.0). Let particle 2 collide into it with velocity (0.4,0.0) from the initial position (3.0, 6.0). Take DT=0.01. Run about 10,000 time step and graph the x-coordinate of both particle every 50 or 100 time-steps. (Can you animate this so that you can see what's going on? Represent each particle by plotting a circle of radius 0.5) Graph also the velocity of both particles. Finally, plot out also the total energy, the kinetic energy, and the potential energy all in one graph. Compared to the initial energy, how accurately is energy conserved? What kind of scattering is being simulated?

2.) Now run your program from a cold start, with N=27, SX=SY=SZ=6.0, by placing particles in a staggered checker-board pattern, with 9 particles in each 3 layers. (If you prefer you may also do a N=64, SX=SY=SZ=8.0 calculation instead.) Use a dt around between 0.005 and 0.01. (Check energy conservation.) Plot the total energy, the kinetic energy, the potential energy and the continuous time average of the kinetic energy all on the same graph as a function of time, for 10,000 to 15,000 time steps. (Note: the kinetic and potential energy should oscillate violently. Also, you don't need to plot it every time step, you can plot every 5 or 10 time steps.) Hand in this plot. How many time steps are required for the average kinetic energy to settle down to a steady value? This is the equilibrium time. Find the corresponding dimensionless temperature T (temperature in units of ϵ/k_B). (For argon, ϵ/k_B=119.8 K)

3.)Difficult After equilibrium, determine the pair correlation function $g(r)$ using a bin size of dr=0.05 as discussed in class. Define an accumulating array $B(nbin)$ with $nbin = 1$ to 100. First, initialize it, by setting all array value to zero

$$B = 0.0 \ .$$

After each update, compute all pair separations r_{ij}. Determine each separation's bin number by setting

$$nbin = INT(r_{ij}/dr) + 1$$

then add to each bin

$$B(nbin) = B(nbin) + 1.0$$

The "pair" density at $r = nbin * dr$ is then given by

$$\rho_p(r) = \frac{B(nbin)}{N * 4\pi(nbin * dr)^2 * dr}$$

and $g(r)$ is given by

$$g(r) = \rho(r)/\rho_b = (V/N) * \rho_p(r)$$

You need to average over many time steps. Hand in this graph of $g(r)$.